6-Benzyl-6,7-dihydro-5H-pyrrolo[3,4-B]pyridine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 178 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.13e-01

Confidence level: 7.82e-01

Nearest Neighbors from the Training Set

Image not found

Mexacarbate
Measured: 302
Predicted: 215

Image not found

Diphenamid
Measured: 209
Predicted: 218

Image not found

Aminocarb
Measured: 100
Predicted: 196

Image not found

Clomazone
Measured: 275
Predicted: 370

Image not found

Dimethirimol
Measured: 89.1
Predicted: 136